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Title: USING THE SCHWINGER VARIATIONAL FUNCTIONAL
FOR THE SOLUTION OF INVERSE TRANSPORT
PROBLEMS

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Form 836 (8/00)

Using the Schwinger Variational Functional for the Solution of Inverse Transport Problems

Based on a paper submitted to
Nuclear Science and Engineering

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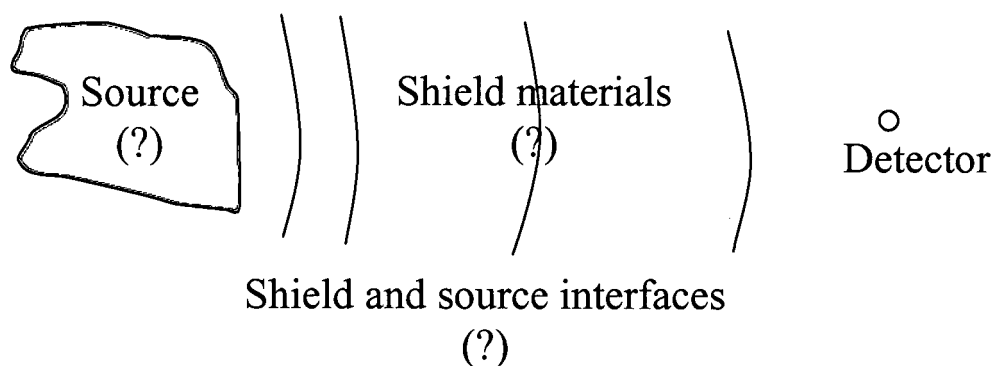


A new iterative inverse method for gamma-ray transport problems is presented. The method, based on a novel application of the Schwinger variational functional, is developed as a perturbation problem in which the current model (in the iterative process) is considered the initial, unperturbed system, and the actual model is considered the perturbed system. The new method requires the solution of a set of uncoupled one-group forward and adjoint transport equations in each iteration. Four inverse problems are considered: determination of 1) interface locations in a multilayer source/shield system; 2) the isotopic composition of an unknown source (including inert elements); 3) interface locations and the source composition simultaneously; and 4) the composition of an unknown layer in the shield. Only the first two problems were actually solved in numerical one-dimensional (spherical) test cases. The method worked well for the unknown interface location problem and extremely well for the unknown source composition problem. Convergence of the method was heavily dependent on the initial guess.

This talk accompanies a full paper of the same title, LA-UR-02-6371.

Motivation

- A direct solution to the Boltzmann transport equation for a known system results in the particle angular or scalar flux somewhere or everywhere in the system, depending on the solution method.
- However, the real problem is frequently the inverse: Given the angular flux or some functional of it (e.g., the particle flux at a detector), what is the system?



- The inverse problem considered here is the determination of
 - + interface locations in a multi-layer source/shield system,
 - + the isotopic composition of an unknown source,
 - + interface locations and source composition, or
 - + the composition of an unknown layer in a shield,

given a set of observed gamma ray fluxes of specific, discrete energies characteristic of the source isotopes.

- The number of unknowns should be less than or equal to the number of observed lines.

- Consider a system that includes some source of gamma rays. The source emits gamma rays at discrete energies, which can be resolved quite well using a high-purity germanium detector. Thus we consider only the transport of photons of discrete energies and assume that any scattered photons lose energy and are removed. The angular flux of photons at the discrete energy denoted by index g is given by

$$\hat{\Omega} \cdot \vec{\nabla} \psi^g(r, \hat{\Omega}) + \Sigma_t^g(r) \psi^g(r, \hat{\Omega}) = q^g(r) \quad (1)$$

for $g = 1, \dots, G$.

- The adjoint equation is

$$-\hat{\Omega} \cdot \vec{\nabla} \psi^{*g}(r, \hat{\Omega}) + \Sigma_t^g(r) \psi^{*g}(r, \hat{\Omega}) = q^{*g}(r) \quad , \quad (2)$$

where the source is to be determined (it will turn out to be the detector response function, as usual).

- These equations can be rendered in operator notation as

$$L^g \psi^g = q^g \quad (3)$$

and

$$L^{*g} \psi^{*g} = q^{*g} \quad . \quad (4)$$

- Suppose the scalar flux for each energy line g is measured at a detector. The quantity of interest is

$$M^g = \int dV \int d\hat{\Omega} \Sigma_d^g(r) \psi^g(r, \hat{\Omega}) \quad , \quad (5)$$

where the detector response function $\Sigma_d^g(r)$ is defined as

$$\Sigma_d^g(r) \equiv \begin{cases} 1 & , \quad r \text{ within the detector volume} \\ 0 & , \quad \text{otherwise} \end{cases} \quad (6)$$

Introducing the inner product notation $\langle \cdot \rangle$ to mean an integral over all phase space (volume and angle), the quantity of interest is

$$M^g = \langle \Sigma_d^g \psi^g \rangle \quad . \quad (7)$$

A weight function or detector efficiency can be built into $\Sigma_d^g(r)$.

- A variational functional for M^g is the Schwinger functional¹

$$M_v^g[\psi^{*g}, \psi^g] = \frac{\langle \Sigma_d^g \psi^g \rangle \langle \psi^{*g} q^g \rangle}{\langle \psi^{*g} L^g \psi^g \rangle} \quad (8)$$

- The variation of M_v^g with respect to ψ^{*g} is

$$\frac{\partial M_v^g}{\partial \psi^{*g}} \delta \psi^{*g} = \frac{\langle \Sigma_d^g \psi^g \rangle \langle \delta \psi^{*g} q^g \rangle}{\langle \psi^{*g} L^g \psi^g \rangle} - \frac{\langle \Sigma_d^g \psi^g \rangle \langle \psi^{*g} q^g \rangle \langle \delta \psi^{*g} L^g \psi^g \rangle}{\langle \psi^{*g} L^g \psi^g \rangle^2}, \quad (9)$$

which is zero for arbitrary and independent variations $\delta \psi^{*g}$ when ψ^g satisfies Eq. (1).

- The variation of M_v^g with respect to ψ^g is

$$\frac{\partial M_v^g}{\partial \psi^g} \delta \psi^g = \frac{\langle \Sigma_d^g \delta \psi^g \rangle \langle \psi^{*g} q^g \rangle}{\langle \psi^{*g} L^g \psi^g \rangle} - \frac{\langle \Sigma_d^g \psi^g \rangle \langle \psi^{*g} q^g \rangle \langle \psi^{*g} L^g \delta \psi^g \rangle}{\langle \psi^{*g} L^g \psi^g \rangle^2}, \quad (10)$$

which is zero for arbitrary and independent variations $\delta \psi^g$ when ψ^{*g} satisfies

$$L^{*g} \psi^{*g} = \Sigma_d^g \quad (11)$$

[as usual, the adjoint source of Eq. (2) is identified as the detector response function].

- In other words, M_v^g is stationary about the functions ψ^g and ψ^{*g} that satisfy Eqs. (3) and (11), respectively, and the stationary value is $M^g = \langle \Sigma_d^g \psi^g \rangle$.

¹ Weston M. Stacey, *Nuclear Reactor Physics*, John Wiley & Sons, Inc., New York, New York, Chap. 13 (2001).

- Suppose the system is perturbed in some way. Then the equations describing the perturbed system are

$$L'^g \psi'^g = q'^g \quad (12)$$

and

$$L'^g \psi'^g = \Sigma_d^g, \quad (13)$$

and the quantity of interest becomes

$$M'^g = \langle \Sigma_d^g \psi'^g \rangle. \quad (14)$$

- A direct estimate of M'^g using the initial, unperturbed flux ψ^g instead of the perturbed flux ψ'^g would be accurate only to first order with respect to the difference $\Delta\psi^g = \psi'^g - \psi^g$.

- The Schwinger functional for M'^g is

$$M'_v{}^g[\psi'^g, \psi'^g] = \frac{\langle \Sigma_d^g \psi'^g \rangle \langle \psi'^g q'^g \rangle}{\langle \psi'^g L'^g \psi'^g \rangle}. \quad (15)$$

- $M'_v{}^g$ is stationary about the functions ψ'^g and ψ'^g that satisfy Eqs. (12) and (13), respectively, and the stationary value is $M'^g = \langle \Sigma_d^g \psi'^g \rangle$.
- Using the initial, unperturbed functions ψ^g and ψ^g instead of the perturbed functions ψ'^g and ψ'^g in $M'_v{}^g$ of Eq. (15) yields an estimate of the perturbed quantity M'^g that is accurate to second order with respect to the differences $\Delta\psi^g = \psi'^g - \psi^g$ and $\Delta\psi^g = \psi'^g - \psi^g$.

Standard application of the Schwinger functional

- Suppose that the configuration of the shielding in the problem is not known exactly, but a reasonable guess is available
 - + That is, the locations of some of the interfaces in the system are not known exactly
- In this case, the guess corresponds to the unperturbed configuration with transport operator L^g and source q^g and the actual system corresponds to the perturbed configuration with transport operator L'^g and source q'^g .
- The forward and adjoint angular fluxes for the guess, ψ^g and ψ^{*g} , are known.
- If L'^g and q'^g were known, then they could be used with trial functions ψ^g and ψ^{*g} in

$$M'_v[\psi^{*g}, \psi^g] = \frac{\langle \Sigma_d^g \psi^g \rangle \langle \psi^{*g} q'^g \rangle}{\langle \psi^{*g} L'^g \psi^g \rangle}$$

[Eq. (15)] to yield an estimate of the flux at the detector that is accurate to second order with respect to the differences $\Delta\psi^g$ and $\Delta\psi^{*g}$.

- Suppose that M'^g , the quantity of interest for the physical system, is known (i.e., the gamma flux for each line has been measured).
- Then Eq. (15) can be used with ψ^g and ψ^{*g} for the guess to arrive at estimates of L'^g and q'^g that describe the physical system.

+ In other words, Eq. (15) can be used with a known $M_v'^g$ and trial functions ψ^g and ψ^{*g} for a model to iteratively improve the model.

- Let the symbol M_o^g represent the measured value and note that

$$\begin{aligned} L'^g &= L^g + \Delta L^g \\ &= L^g + \Delta \Sigma_t^g \end{aligned} \quad (16)$$

and

$$q'^g = q^g + \Delta q^g \quad (17)$$

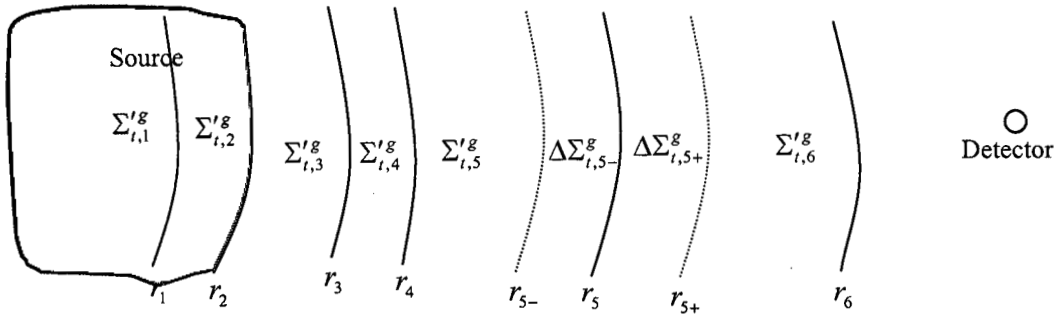
- Using the measured value for $M_v'^g$, trial functions ψ^g and ψ^{*g} for ψ'^g and ψ'^{*g} , and Eqs. (16) and (17), Eq. (15) becomes

$$M_o^g = \frac{\langle \Sigma_d^g \psi^g \rangle [\langle \psi^{*g} q^g \rangle + \langle \psi^{*g} \Delta q^g \rangle]}{\langle \psi^{*g} L^g \psi^g \rangle + \langle \psi^{*g} \Delta \Sigma_t^g \psi^g \rangle} \quad (18)$$

Rearranging yields

$$\frac{1}{\langle \psi^{*g} q^g \rangle} \left[\langle \psi^{*g} \Delta \Sigma_t^g \psi^g \rangle - \frac{M_o^g}{M_o^g} \langle \psi^{*g} \Delta q^g \rangle \right] = \frac{M_o^g - M_o^g}{M_o^g}, \quad g = 1, \dots, G \quad (19)$$

- The right side of Eq. (19) is the relative difference between the measured detector flux of line g and that computed using the assumed (unperturbed) model.
- $\Delta \Sigma_t^g$ and Δq^g , or the integrals containing them, are unknown



- The cross-section integral in Eq. (19) becomes

$$\begin{aligned} \langle \psi^{*g} \Delta \Sigma_t^g \psi^g \rangle = \sum_{n=1}^N \left[\int_{r_{n-}}^{r_n} dV \int d\hat{\Omega} \psi^{*g} \Delta \Sigma_{t,n-}^g \psi^g H(r_n - r'_n) \right. \\ \left. + \int_{r_n}^{r_{n+}} dV \int d\hat{\Omega} \psi^{*g} \Delta \Sigma_{t,n+}^g \psi^g H(r'_n - r_n) \right], \end{aligned} \quad (20)$$

where N is the number of boundaries.

- Define

$$\Delta \Sigma_{t,n}^g \equiv \Delta \Sigma_{t,n+}^g = -\Delta \Sigma_{t,n-}^g. \quad (21)$$

- Using $\Delta \Sigma_{t,n}^g$ and identifying r'_n as the location of the perturbed boundary r_{n-} or r_{n+} , Eq. (20) yields

$$\langle \psi^{*g} \Delta \Sigma_t^g \psi^g \rangle = \sum_{n=1}^N \Delta \Sigma_{t,n}^g \underbrace{\int_{r_n}^{r'_n} dV \int d\hat{\Omega} \psi^{*g} \psi^g}_{I_n^g(r'_n)} \quad (22)$$

- The same can be done for the source integral in Eq. (19):

$$\langle \psi^{*g} \Delta q^g \rangle = \sum_{n=1}^{N_s} \Delta q_n^g \underbrace{\int_{r_n}^{r'_n} dV \int d\hat{\Omega} \psi^{*g}}_{I_{s,n}^{*g}(r'_n)} \quad (23)$$

- Let the index n be over unknown interface locations only

- $$\frac{1}{\langle \psi^{*g} q^g \rangle} \left[\langle \psi^{*g} \Delta \Sigma_t^g \psi^g \rangle - \frac{M_o^g}{M_o^g} \langle \psi^{*g} \Delta q^g \rangle \right] = \frac{M^g - M_o^g}{M_o^g}, \quad g = 1, \dots, G$$

[Eq. (19)] becomes

$$\frac{1}{\langle \psi^{*g} q^g \rangle} \left[\sum_{n=1}^N \Delta \Sigma_{t,n}^g I_n^g(r'_n) - \frac{M_o^g}{M_o^g} \sum_{n=1}^{N_s} \Delta q_n^g I_{s,n}^{*g}(r'_n) \right] = \frac{M^g - M_o^g}{M_o^g}. \quad (24)$$

There are G equations and $G \times N$ unknowns $I_n^g(r'_n)$ and $I_{s,n}^{*g}(r'_n)$. We must rewrite Eq. (24) for the unknown r'_n directly.

- Expand $I_n^g(r'_n)$ and $I_{s,n}^{*g}(r'_n)$ each in a Taylor series about r_n :

$$I_n^g(r'_n) = I_n^g(r_n) + \left. \frac{\partial I_n^g(r)}{\partial r} \right|_{r=r_n} (r'_n - r_n) + \frac{1}{2} \left. \frac{\partial^2 I_n^g(r)}{\partial^2 r} \right|_{r=r_n} (r'_n - r_n)^2 + \dots \quad (25)$$

- Noting that the zero'th order term in each expansion is identically zero, neglecting the second- and higher-order terms, and using the result in Eq. (24) yields

$$\frac{1}{\langle \psi^{*g} q^g \rangle} \left[\sum_{n=1}^N \Delta \Sigma_{t,n}^g \left. \frac{\partial I_n^g(r)}{\partial r} \right|_{r=r_n} \Delta r_n - \frac{M_o^g}{M_o^g} \sum_{n=1}^{N_s} \Delta q_n^g \left. \frac{\partial I_{s,n}^{*g}(r)}{\partial r} \right|_{r=r_n} \Delta r_n \right] = \frac{M^g - M_o^g}{M_o^g} \quad (26)$$

- Equation (26) can be recast as a matrix equation:

$$\underline{\underline{R}} \underline{\underline{\Delta r}} = \underline{\underline{P}} \quad (27)$$

where $\underline{\underline{R}}$ is a $G \times N$ matrix, $\underline{\underline{P}}$ is a $G \times 1$ vector, and $\underline{\underline{\Delta r}}$ is an $N \times 1$ vector.

- Equation (27) can be solved as long as the number of unknown boundaries, N , is less than or equal to the number of observed lines, G . The shape of the unknown boundaries must be known, although they needn't be analytic surfaces.

- Let there be only one homogeneous and isotopic source region
- The integrals in Eq. (19) are

$$\langle \psi^{*g} \Delta \Sigma_t^g \psi^g \rangle = \Delta \Sigma_{t,s}^g \underbrace{\int_{V_s} dV \int d\hat{\Omega} \psi^{*g} \psi^g}_{I_s^g} \quad (28)$$

and

$$\langle \psi^{*g} \Delta q^g \rangle = \Delta q^g \underbrace{\int_{V_s} dV \int d\hat{\Omega} \psi^{*g}}_{I_s^{*g}} \quad (29)$$

- Equation (19) becomes

$$\frac{1}{\langle \psi^{*g} q^g \rangle} \left[\Delta \Sigma_{t,s}^g I_s^g - \frac{M^g}{M_o^g} \Delta q^g I_s^{*g} \right] = \frac{M^g - M_o^g}{M_o^g} \quad (30)$$

- Write $\Delta \Sigma_{t,s}^g$ and Δq^g in terms of the source weight fractions. Eq. (30) becomes

$$\frac{\rho_s N_A}{\langle \psi^{*g} q^g \rangle} \left[I_s^g \sum_{j=1}^J \frac{\sigma_{t,j}^g}{A_j} \Delta f_j - \frac{M^g}{M_o^g} \frac{q_i^g}{A_i} I_s^{*g} \Delta f_i \right] = \frac{M^g - M_o^g}{M_o^g} \quad (31)$$

- Equation (31) can be recast as a matrix equation:

$$\underline{\underline{F}} \underline{\Delta f} = \underline{P} \quad (32)$$

where $\underline{\underline{F}}$ is a $G \times J$ matrix, \underline{P} is a $G \times 1$ vector, and $\underline{\Delta f}$ is an $J \times 1$ vector.

- Equation (32) can be solved as long as the number of unknown weight fractions, J , is less than or equal to the number of observed lines, G .
- Note especially that this method can be used to find the weight fractions of source isotopes and inert elements (such as stable oxygen)

Two other applications

- Identification of unknown interface locations *and* unknown source composition:

$$\begin{aligned}
 & \frac{\rho_s N_A}{\langle \psi^{*g} q^g \rangle} \left\{ I_s^g \sum_{j=1}^J \frac{\sigma_{t,j}^g}{A_j} \Delta f_j + \frac{\partial I_1^g(r)}{\partial r} \Big|_{r=r_s} \left(\sum_{j=1}^J \frac{\sigma_{t,j}^g}{A_j} \Delta f_j \right) \Delta r_s + \frac{1}{\rho_s N_A} \frac{\partial I_1^g(r)}{\partial r} \Big|_{r=r_s} (\Sigma_{t,s}^g(\underline{f}) - \Sigma'_{t,2}^g) \Delta r_s \right. \\
 & + \frac{1}{\rho_s N_A} \sum_{n=2}^N \Delta \Sigma_{t,n}^g \frac{\partial I_n^g(r)}{\partial r} \Big|_{r=r_n} \Delta r_n - \frac{M^g}{M_o^g} \left[I_s^{*g} \sum_{j=1}^J \frac{q_j^g}{A_j} \Delta f_j + \frac{\partial I_{s,1}^{*g}(r)}{\partial r} \Big|_{r=r_s} \left(\sum_{j=1}^J \frac{q_j^g}{A_j} \Delta f_j \right) \Delta r_s \right. \\
 & \left. \left. + \frac{1}{\rho_s N_A} \frac{\partial I_{s,1}^{*g}(r)}{\partial r} \Big|_{r=r_s} q^g(\underline{f}) \Delta r_s \right] \right\} = \frac{M^g - M_o^g}{M_o^g}, \quad g = 1, \dots, G \quad (33)
 \end{aligned}$$

- Identification of unknown layers in the shield:

$$\sum_{n=1}^N \Sigma'_{t,n}^g I_n^g = \frac{M^g - M_o^g}{M_o^g} + \sum_{n=1}^N \Sigma_{t,n}^g I_n^g, \quad g = 1, \dots, G \quad (34)$$

+ There are G equations and $G \times N$ unknowns $\Sigma'_{t,n}^g$. Thus, Eq. (34) is not solvable unless there is only one unknown material in the shield, in which case:

$$\Sigma'_{t,1}^g = \frac{1}{I_1^g} \frac{M^g - M_o^g}{M_o^g} + \Sigma_{t,1}^g, \quad g = 1, \dots, G \quad (35)$$

+ These equations are uncoupled

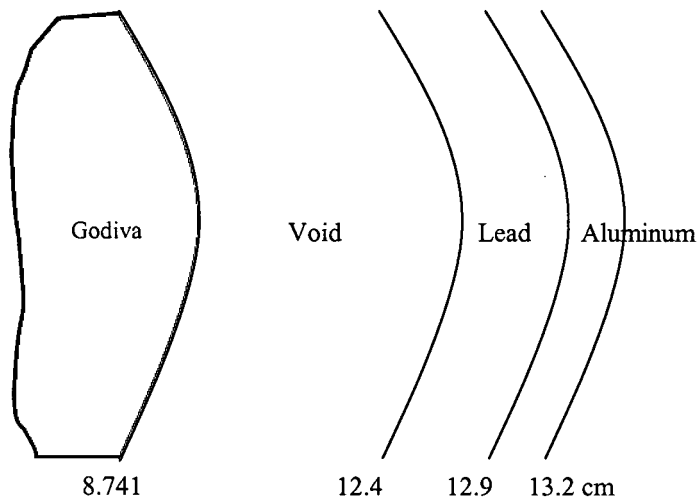
+ Identification of the composition of the unknown shield layer may be achieved using photon cross section tables when the $\Sigma'_{t,1}^g$ have been determined.

Implementation

- The general algorithm for implementation of the new method is as follows:
 1. Use available data to generate an initial model. The model has either a few unknown interface locations in the source and/or shield, or a few unknown isotopic weight fractions in the source, or unknown interface locations and unknown source isotopic weight fractions, or one unknown layer in a multilayer shield.
 2. Compute the angular flux ψ^g and the detector response M^g for each line for the model. If the differences between M^g and the measured values M_o^g are large, go to step 3. If the differences are acceptably small, go to step 6.
 3. Compute ψ^{*g} and construct the left side of Eq. (19) as developed in this talk. Construct the right side of Eq. (19) using the computed and measured detector responses.
 4. Solve for the change in the interface locations Δr , or for the change in the source isotopic weight fractions Δf , or for Δr and Δf , or for the shield layer cross sections $\Sigma'_{t,1}^g$. Update the radii and/or weight fraction vectors.
 5. Using the new values from step 4, construct an updated operator L^g and return to step 2.
 6. Done.
- The one-group forward and adjoint transport calculations can be performed with either deterministic or Monte Carlo methods. Photon cross sections can be constructed from the continuous-energy MCNP library MCPLIB02
- The method was implemented to solve the unknown interface location problem and the unknown source composition problem in one-dimensional (spherical) geometry
- Problem of nonphysical results.

Test cases

- Test cases used a spherical Godiva model (94.73% ^{235}U and 5.27% ^{238}U , mass density of 18.74 g/cm^3) in a lead/aluminum shield and a 6%-enriched UO_2 (mass density 10.5 g/cm^3) nuclear reactor fuel model in the same shield



- Uranium gamma lines:

Isotope	Line Energy (keV)	Specific Intensity ($\gamma/\text{s/atom}$)
^{235}U	144.0	3.297×10^6
^{235}U	186.0	1.728×10^7
^{238}U	766.0	1.525×10^4
^{238}U	1001.0	4.033×10^4

- The discrete-ordinates code PARTISN was used for the forward and adjoint transport calculations. S_8 gamma transport was used.
- “Measurements” were obtained with S_8 calculations

Test cases: Unknown interface locations

- Results for Unknown Interface Test Problems^a

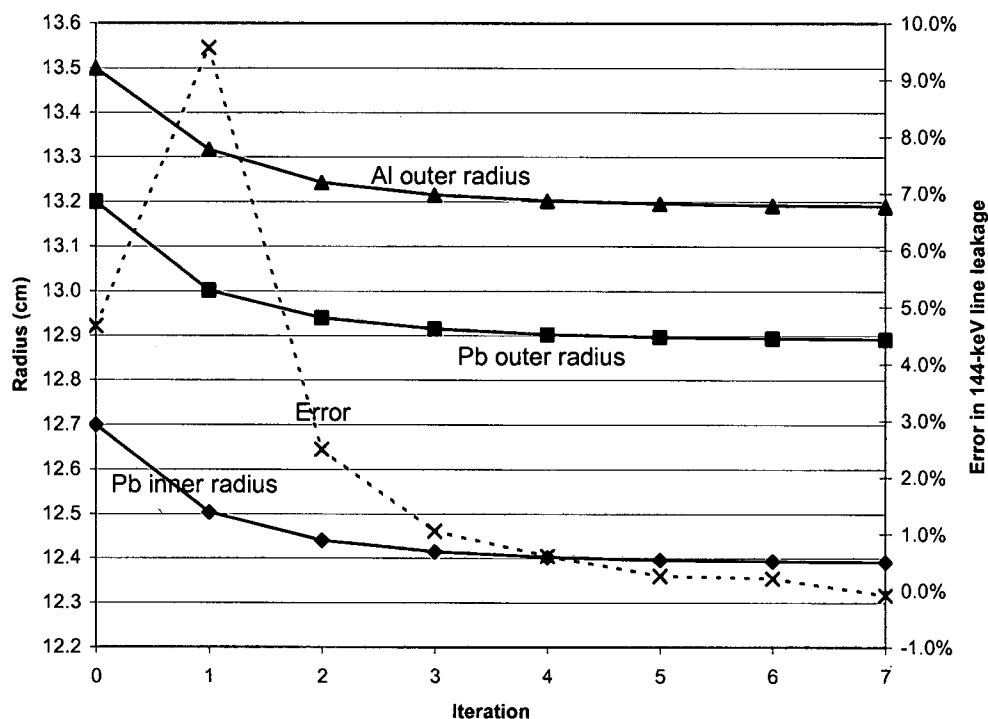
Descriptor	Model	Outer Radii ^a			
		Godiva	Void	Lead	Aluminum
Actual Model		8.7410	12.4000	12.9000	13.2000
Case 1a	Initial	8.741	12.1	12.6	12.9
	Converged	8.741	12.3856	12.8856	13.1836
Case 1b	Initial	8.741	12.7	13.2	13.5
	Converged	8.741	12.3916	12.8916	13.1902
Case 1c	Initial	8.741	14.4	14.9	15.2
	Converged	Did Not Converge			
Case 2a	Initial	8.741	12.3	12.6	15.0
	Converged	Did Not Converge			
Case 2b	Initial	8.741	12.0	12.6	15.0
	Converged	8.741	12.3916	12.8916	13.1902
Case 3a	Initial	9.0	12.0	12.6	13.2
	“Converged”	9.0	12.1066	12.6	13.2
Case 3b	Initial	9.0	12.1066	12.6	13.2
	Converged	8.7619	12.3893	12.8891	13.2

^aItalics represent quantities that are known or assumed known.

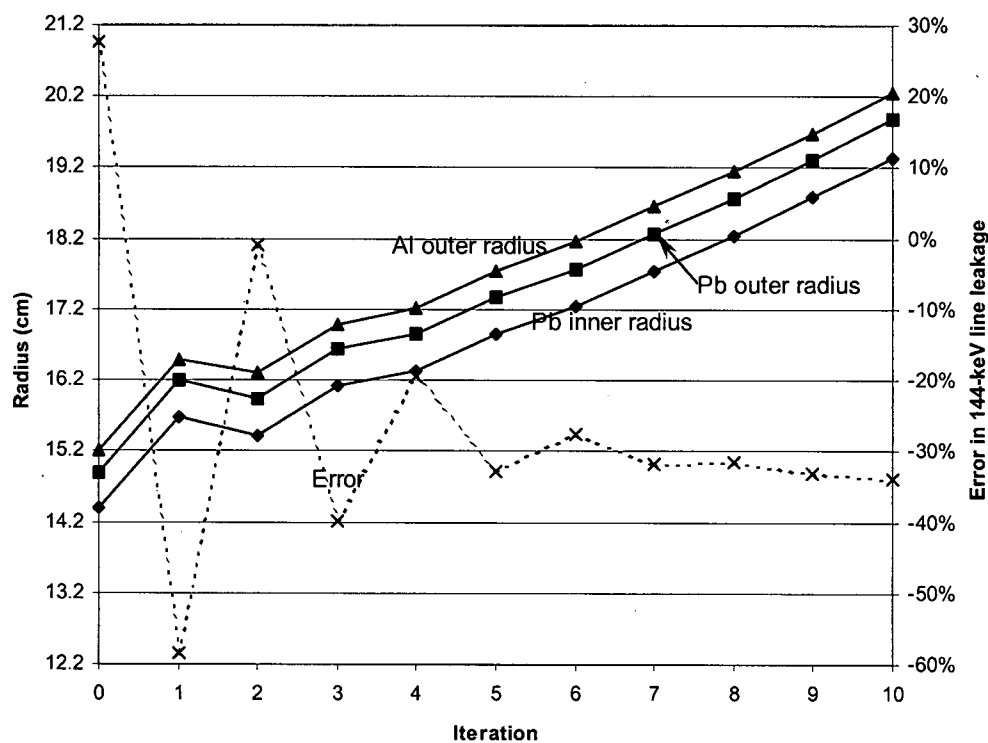
- Convergence is sensitive to the initial model.

Iterations for unknown interface location test cases

- Iterations for case 1b:



- Iterations for case 1c:



Test cases: Unknown source composition

- Results for Unknown Source Composition Test Problems

Descriptor	Model	Source Material Weight Fractions			
		²³⁵ U	²³⁸ U	O	Gd
Case 4	Actual	0.947300	0.0527000	—	—
	Initial	0.1	0.9	—	—
	Converged	0.947279	0.0527214	—	—
Case 5	Actual	0.0528860	0.828544	0.118570	—
	Initial	0.3333333	0.333333	0.333333	—
	Converged	0.0528629	0.828511	0.118626	—
Case 6 6a	Actual	0.0502420	0.787117	0.112641	0.0500000
	Initial	0.25	0.25	0.25	0.25
	Converged	Did Not Converge			
6b	Initial	0.50	0.166666	0.166666	0.166666
	Converged	0.0502345	0.786633	0.113696	0.0494363

- Convergence is sensitive to the initial model.
- Convergence in these problems is very fast: one or two iterations

Summary and conclusions

- A new iterative inverse method for gamma-ray transport problems has been presented.
- The method, based on a novel application of the Schwinger variational functional, is developed as a perturbation problem in which the current model (in the iterative process) is considered the initial, unperturbed system, and the actual model is considered the perturbed system.
- The method worked well for the unknown interface location problem and extremely well for the unknown source composition problem.
- Convergence of the method was heavily dependent on the initial guess.
- Future work: Incorporate constraints into the variational formalism
 - + Constraints that would exclude nonphysical solutions such as negative interface locations or weight fractions would be of great benefit.
 - + It would also be helpful to develop constraints that would directly incorporate knowledge of the system beyond simply whether an interface location or source weight fraction is known or unknown. For example, the known mass or thickness of a shield layer cannot presently be used in the inverse method to update the unknown parameters.
- Future work: Implement the method with continuous-energy Monte Carlo transport calculations
- Future work: Actual measurements (or Monte Carlo simulations)